University of California at San Diego – Department of Physics – Prof. John McGreevy

Physics 239 Spring 2016
Assignment 2

Due 11am Tuesday, April 19, 2016

1. **Entanglement entropy in a quantum not-so-many-body system.** [from Tarun Grover]

   Consider a system consisting of two electrons, each with spin one-half, and each of which can occupy either of two sites labelled $i = 1, 2$. The dynamics is governed by the following (Hubbard) Hamiltonian:

   $$\mathbf{H} = -t \sum_{\sigma=\uparrow,\downarrow} \left(\mathbf{c}^\dagger_{1\sigma} \mathbf{c}_{2\sigma} + \mathbf{c}^\dagger_{2\sigma} \mathbf{c}_{1\sigma} \right) + U \sum_i \mathbf{n}_{i\uparrow} \mathbf{n}_{i\downarrow}.$$

   $\sigma =\uparrow, \downarrow$ labels the electron spin. $\mathbf{c}$ and $\mathbf{c}^\dagger$ are fermion creation and annihilation operators,

   $$\{\mathbf{c}_{i\sigma}, \mathbf{c}^\dagger_{i'\sigma'}\} = \delta_{ii'}\delta_{\sigma\sigma'}$$

   and $\mathbf{n}_{i\sigma} \equiv \mathbf{c}^\dagger_{i\sigma}\mathbf{c}_{i\sigma}$ is the number operator. The condition that there is a total of two electrons means we only consider states $|\psi\rangle$ with

   $$\left(\sum_{i,\sigma} \mathbf{n}_{i\sigma} - 2 \right) |\psi\rangle = 0.$$

   The first term is a kinetic energy which allows the electrons to hop between the two sites. The second term is a potential energy which penalizes the states where two electrons sit at the same site, by an energy $U > 0$.

   (a) Enumerate a basis of two-electron states (make sure they satisfy the Pauli exclusion principle).

   (b) The Hamiltonian above has some symmetries. In particular, the total electron spin in the $\hat{z}$ direction is conserved. For simplicity, let's focus on the states where it is zero, such as $\mathbf{c}^\dagger_{1\uparrow}\mathbf{c}^\dagger_{2\downarrow}|0\rangle$ where $|0\rangle$ is the state with no electrons, $\mathbf{c}_{i\sigma}|0\rangle = 0$. Find a basis for this subspace, $\{\phi_a\}, a = 1..N$.

   (c) Find the matrix elements of the Hamiltonian in this basis,

   $$h_{ij} \equiv \langle \phi_a | \mathbf{H} | \phi_b \rangle, \quad a, b = 1..N.$$

(d) Find the eigenstate and eigenvalue of the matrix h with the lowest eigenvalue. Write the groundstate as

$$|\Psi\rangle = \sum_{a=1}^{N} \alpha_a |\phi_a\rangle .$$

(e) Before imposing the global constraints on particle number and S^z, the Hilbert space can be factored (up to some signs because fermions are weird) by site: $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$, where $\mathcal{H}_i = \text{span}\{|0\rangle, \mathbf{c}_{i\uparrow}^\dagger |0\rangle, \mathbf{c}_{i\downarrow}^\dagger |0\rangle, \mathbf{c}_{i\uparrow}^\dagger \mathbf{c}_{i\downarrow}^\dagger |0\rangle\}$. Using this bipartition, construct the reduced density matrix for the first site in the groundstate:

$$\boldsymbol{\rho}_1 \equiv \text{tr}_{\mathcal{H}_2} |\Psi\rangle \langle\Psi| .$$

(f) Find the eigenvalues λ_α of $\boldsymbol{\rho}_1$. Calculate the von Neumann entropy of $\boldsymbol{\rho}_1$, $S(\boldsymbol{\rho}_1) = -\sum_\alpha \lambda_\alpha \log \lambda_\alpha$ as a function of U/t. What is the numerical value when $U/t \to \infty$?

(g) **Super-Exchange.** Go back to the beginning and consider the limit $U \gg t$. What are the groundstates when $U/t \to \infty$, so that we may completely ignore the hopping term?

At second order in degenerate perturbation theory, find the effective Hamiltonian which splits the degeneracy for small but nonzero t/U. Write the answer in terms of the spin operator

$$\vec{\mathbf{S}}_i \equiv \mathbf{c}_{i\sigma}^\dagger \vec{\sigma}_{\sigma\sigma'} \mathbf{c}_{i\sigma'}.$$

The sign is important!

(h) Redo all the previous parts for the case where the two particles are spin-half bosons,

$$\mathbf{c}_{i\sigma} \rightsquigarrow \mathbf{b}_{i\sigma}, \quad [\mathbf{b}_{i\sigma}, \mathbf{b}_{i'\sigma'}^\dagger] = \delta_{ii'}\delta_{\sigma\sigma'}.$$

2. **Chain rules.**

Show that for a joint distribution of n random variables $p(X_1 \cdots X_n)$, the joint and conditional entropies satisfy the following chain rule:

$$H(X_1 \cdots X_n) = \sum_{i=1}^{n} H(X_i | X_{i-1} \cdots X_1).$$

Show that the $n = 2$ case is the expectation of the log of the BHS of Bayes rule. Then repeatedly apply the $n = 2$ case to increasing values of n.

3. **Learning decreases ignorance only on average.**

Consider the joint distribution $p_{yx} = \begin{pmatrix} 0 & a \\ b & b \end{pmatrix}_{yx}$, where $y = \uparrow, \downarrow$ is the row index and $x = \uparrow, \downarrow$ is the column index (so yx are like the indices on a matrix). Normalization implies $\sum_{xy} p_{xy} = a + 2b = 1$, so we have a one-parameter family of distributions, labelled by b.

What is the allowed range of b?

Find the marginals for x and y. Find the conditional probabilities $p(x|y)$ and $p(y|x)$.

Check that $H(X|Y) \leq H(X)$ and $H(Y|X) \leq H(Y)$ for any choice of b.

Show, however, that $H(X|Y = \downarrow) > H(X)$ for any $b < \frac{1}{2}$.